Annot Documentation

Release 0.2

bue

July 02, 2015

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Annot is a web application to annotate bioscience experiments, to capture the experiments metadata and data so that data are ready for analysis and sharing.

Annot is utterly modularly implemented to be adaptable to each laboratories specific needs.

Annot is written in Python 3 with Django.

The source code is distributed under the free and open source GNU AGPLv3 license, while this documentation is under the free and open source GNU FDLv1.3 license.

Contents:

CHAPTER 1

Introduction

1.1 Preface

In the past two decades, technological developments have made it feasible to generate large volumes of heterogeneous biological data. Bioinformatics is an interdisciplinary field that develops methods and software tools for understanding and mining these large-scale and complex biological data. A major challenge in bioinformatics is the integration of data from different sources. Several efforts have been made to aid in this process, including: standard metadata annotation formats to share and describe the experiments (ISA-Tab), minimal information guidelines to report biological and biomedical science (MIBBI project) and biological and biomedical ontology-based controlled vocabulary (OBO Foundry and Bioontology). However, the bioinformatics community still struggles to bring these standards, guidelines, and ontologies into the wet laboratory, the workbench where the biological experiments are carried out.

1.2 Why Annot?

Wet lab scientists use their lab books or traditional laboratory information management systems to keep track of the samples, reagents, assay workflow, provenance of results, and to record data. These interactions are usually focused on human beings, not machines. Consequently, as every **bioinformatician** knows, when sophisticated data analysis or data integration should be done, the data usually have to be "scrubbed" to be usable by computers. Unfortunately, this process is time-consuming and error-prone.

A major part of the problem is the lack adherence to a controlled vocabulary to annotate data of biological experiments. Even though annotating experiments with a controlled vocabulary would reduce common data integration errors, constant compliance is difficult to achieve using standard operating procedures.

Here we introduce Annot, a web application to bridge the gap between wet lab scientists and data analysts. Annot is a web application to captures the metadata, raw data, and processed data from biological studies in standardized computational formats so that they are ready for analysis and sharing.

1.3 Implementation

The foundation of Annot lies in the controlled vocabulary. Whenever possible, we derive controlled vocabulary from established ontologies that can be easily updated to the latest ontology version and extended to include missing terms. Internal terms then never interfere with official ontology terms. Each controlled vocabulary is handled as a django application.

Wet lab scientists had input on the structure of the **assay building bricks** (symbolized by the jigsaw pieces). Whenever possible, we adhered to the actual LINCs metadata standard and ISA-Tab specification.

Assay workflows can be connected by the assay building bricks analogous to a Unix pipeline, to track data provenance. This Lego-like building brick system makes it easy to keep the workflow up-to-date with actual assay development in the wet lab or add new assay workflows.

Overall, the system's goal is to be modular, adaptable, lean and agile but focused on the major task: capturing biological study metadata and data annotations so that data are ready for analysis and sharing.

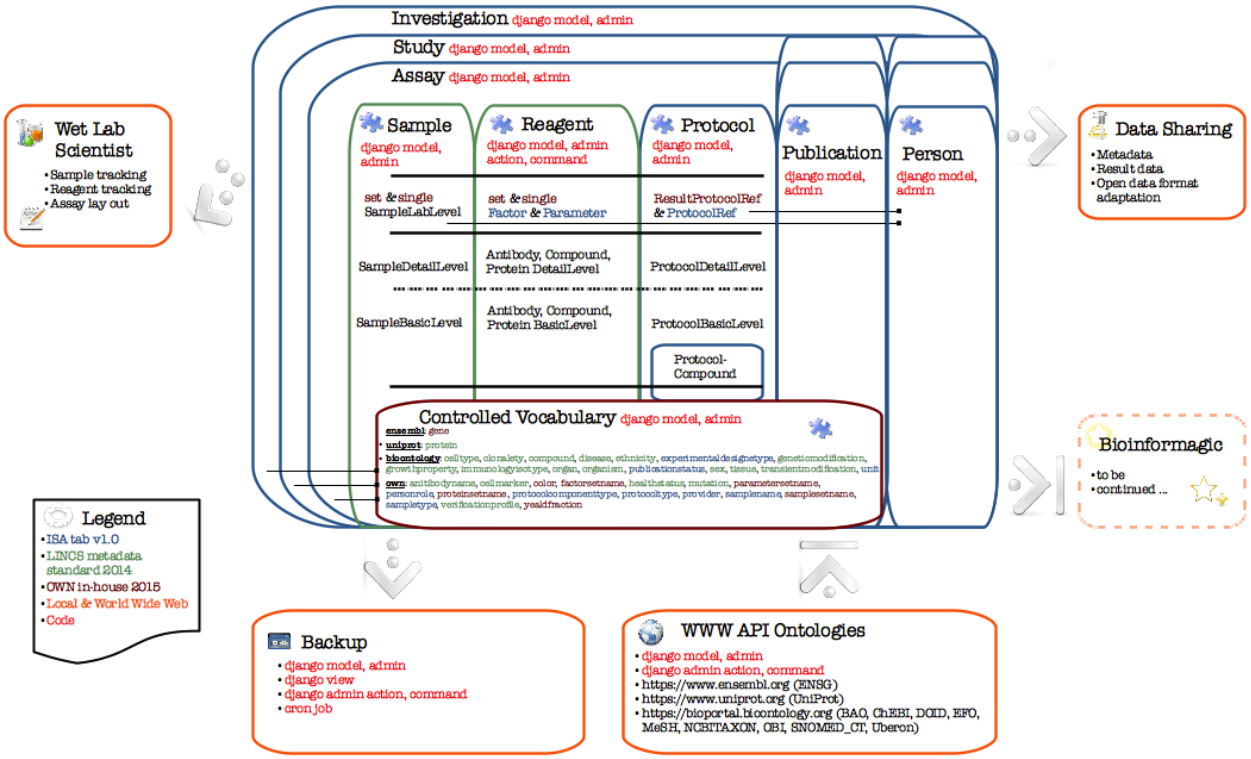

Figure: Blueprint for the Annot interfaces and the modular Annot django project architecture. Investigation, study, assays, person, publication, protocol, reagent types, sample and each vocabulary are handled by a separate django application, represented by nested rectangles.

1.4 Source Code

The source code is distributed under the free and open source AGPLv3 license through https://gitlab.com/biotransistor/annot .

Annot is written in Python 3.4, utilizing the Django 1.8 web framework with PostgreSQL 9.4 and Apache 2.4. Annot is to deployed with the Docker 1.6 distribution platform. All images are based on the officil Debian 8 Jessie base image. Early development and deployment evolved by running a FreeBSD 10 operating system in a virtual machine.

1.5 Project References

PyCon 2015 Montreal: https://us.pycon.org/2015/schedule/presentation/461/

CHAPTER 2

User Manual

This manual is intended for the user of Annot. First this manual will cover how-to install and run Annot for your lab or you self. Second this manual will describe all graphical user interface (GUI) features implemented.

2.1 How-to Get Annot Up and Running

2.1.1 Install Annot

1. **Install Docker on the machine you would like to run Annot for you lab.** Docker is able runs on Linux, Mac OSX, MS Windows and many of cloud platform flavors.
2. Fetch the latest Annot related Docker images, hosted at Docker hub, by running the docker pull commands. All docker images downloaded to your local computer can be listed running the docker images command.

```
docker pull elmar/annot
docker pull elmar/media_annot
docker pull elmar/apache_annot
docker images
```

3. Generate a bioontology.org BioPortal account. Go to your BioPortal account settings to figure out your application interface (API) key.
4. Write a plain text crowbar.py with the following content. Adapt the content inside the double quotes:

```
SECRET_KEY = "about_64_characters_long`~!@#$%^&*()-+=:;<,>.?/"
DATABASE_PASSWORD = "annot_postgresql_database_password"
APIKEY = "your_BioPortal_bioontology.org_API_key"
CONTACT = "you@emailadress"
```

5. Build the Docker container out of the fetched images. Adapt */path/to/crowbar.py* and */path/to/backupfolder* in the last docker run command below to your settings. If you have to choose an other port then 80, choose a port between 49152 and 65535. For the rest of this documentation we assume Annot to run on port 52872, as specified by the last docker run command.

```
docker run --name=annot elmar/annot /bin/true
docker run --name=media_annot elmar/media_annot /bin/true
docker run --name=apache_annot --volumes-from=annot -v=/path/to/crowbar.py:/var/www/annot/prjann
```

6. Runnig docker ps -a and docker ps you will figure out that the annot web application, which runs in the apache_annot docker container, is already started. In future you can start and stop the annot web application with the docker start and stop command. When you run docker start apache_annot be patient. It may take a

while till the container is booted and listed at docker ps. For a working web application don't forget to start the postgresql daemon too, as explained further below.

```
docker ps -a
docker ps
docker start apache_annot
docker stop apache_annot
```

7. Figure out the hostname or IP address from the machine you are running docker. The way how to do this depends on the operating system docker is runing. Check out the Docker installation documentation for detailed informaton how to do this. For the rest of the documentation we assume IP address 127.0.0.1 .
8. Enter apache_annot. Run on the command line:

```
docker exec -ti apache_annot /bin/bash
```

1. Inside apache_annot check if the postgresql database daemon is running. Start if necessary.

```
/etc/init.d/postgresql status
/etc/init.d/postgresql start
```

2. Indside apache_annot create Postgresql annot user and annot database. Execute the commands one by one! Answer the posed questions. For the annot user utilize same password as specified in the cowbar.py file before.

```
su postgres
createdb annot
createuser -P annot
psql -U postgres -d annot -c"GRANT ALL PRIVILEGES ON DATABASE annot TO annot;"
exit
```

3. Inside apache_annot set up the annot project. Execute the commands one by one!

```
chown www-data:root -R /var/www/media
cd /var/www/annot/
python3 demigrations.py
python3 manage.py makemigrations
python3 manage.py migrate
python3 manage.py createsuperuser
python3 manage.py collectstatic
exit
```

9. Fire up you favorite web browser - we recommend mozilla's Firefox - and surf to the place where Annot is running. In this documentation we assume Annot is running in IP address 127.0.0.1 port 52872. Write into the browsers address bar:

```
http://127.0.0.1:52872/admin/
```

10. Log in with the above generated superuser credential.

That's all.

CHAPTER 3

Developer Manual

This manual is intended for programers who would like to take part in the Annot project code development or adapt the Annot source code to their needs.

You can skip step 4 and straight git clone git@gitlab.com:biotransistor/annot.git without forking, if you only like to adapt the Annot source code to your needs and not plane to fork you changes back to the Annot project master branch.

3.1 How-to Get Annot Developer Version Up and Running

3.1.1 Install Annot for Development

1. **Install Docker on the computer you would like to run Annot for development. (This can be the same at the computer whe**
   Docker is able to run on Linux, Mac OSX, MS Windows and many cloud platform flavors.
2. Fetch the latest Annot related Docker images, hosted at Docker hub, by running the docker pull commands. All docker images downloaded to your local computer can be listed running the docker images command.

```
docker pull elmar/media_annot
docker pull elmar/apache_annot
docker images
```

3. On the development computer install Git. How will depend on the flavor of the operating system you are running.
4. Get the Annot source code

1. Sign in at GitLab, sign up if you not already have an account. If you not already have done so, generate an ssh-key at your development computer and load the public ssh-key up to your GitLab account.
2. Fork from https://gitlab.com/biotransistor/annot the master branch.
3. Clone from your fork. In the example below replace *your_namespace* with your GitLab username. This example would clone from the master branch of your fork.

```
git clone git@gitlab.com:your_namespace/annot.git
```

5. Generate a bioontology.org BioPortal account. Go to your BioPortal account settings to figure out your application interface (API) key.
6. Write a plain text crowbar.py with the following content. Adapt the content inside the double quotes:

```
SECRET_KEY = "about_64_characters_long`~!@#$%^&*()-+=:;<,>.?/"
DATABASE_PASSWORD = "annot_postgresql_database_password"
APIKEY = "your_BioPortal_bioontology.org_API_key"
CONTACT = "you@emailadress"
```

7. Build the Docker containers out of the fetched images and the cloned source code. Adapt */path/to/annot*, */path/to/crowbar.py* and */path/to/backupfolder* in the last docker run command below to your settings. If you have to choose an other port then 80, choose a port between 49152 and 65535. For the rest of this documentation we assume Annot to run on port 35627, as specified by the last docker run command.:

```
docker run --name=media_annotdev elmar/media_annot /bin/true
docker run --name=apache_annotdev -v=/path/to/annot:/var/www/annot -v=/path/to/crowbar.py:/var/w
```

8. Container with continuer with *step 6 of the User Manual Install Annot* instruction.

3.1.2 Run Annot for Development

- To work on the source code open a terminal. If the host server where apache_annotdev is running is not your local machine, ssh into the host server. cd into the annot directory cloned before. Changes to the source code will immediately take effect. Hint: if the host is not your local computer ssh into the host server to work with the source code.
- Open an other shell. Enter apache_annot to control the apache web server. The following commands might be of use:

```
docker exec -ti apache_annotdev /bin/bash

/etc/init.d/postgresql
/etc/init.d/postgresql status
/etc/init.d/postgresql start
/etc/init.d/postgresql restart
/etc/init.d/postgresql stop

/etc/init.d/apache2
/etc/init.d/apache2 status
/etc/init.d/apache2 start
/etc/init.d/apache2 restart
/etc/init.d/apache2 stop
```

- Don't forget to add, commit, and push your changes to your git repository. And if your code runs, don't forget to merge request that the changes can be forked back into the official repository.

CHAPTER 4

Epilog

4.1 Author List

In alphabetic order:

Amanda Esch: wet lab knowledge antibody
Carly King: documentation work
Damir Sudar: concept input
David Kilburn: concept input
Derrick Hee: programmer cron job
Elmar Bucher (bue): programmer main
Jim Korkola: wet lab knowledge MEMA assay
Joe Gray: principal investigator
Laura Heiser: principal investigator
Mark Dane: concept input
Michel Nederlof: concept input
Nicholas Wang : concept input
Rebecca Smith: wet lab knowledge protein and compounds
Tiera Liby: wet lab knowledge biological samples
Wally Thompson: wet lab knowledge protein and compounds

4.1.1 Who is Author?

It does not matter if you contributed to the project by code or documentation, when your fork is ready to be merged with the official master branch add your self to the author list! There are as well a view authors that have not contributed by code or documentation, but by conceptual input or by biological wet lab knowledge which was important to the project.

4.2 Aknowledgement

This work was supported by the NIH LINCS center grant 1U54HG008100 to J.W.G.

CHAPTER 5

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Version 3, 19 November 2007

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CHAPTER 6

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CHAPTER 7

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